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Signal Processing for Time-Series Functions on a Graph

by Humberto Muñoz-Barona, Jean Vettel, and
Addison Bohannon

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Signal Processing for Time-Series Functions on a Graph

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1. Introduction

In many real-world systems, the most interesting behavior emerges from complex interactions between the constituent elements.¹ These systems arise in applications as varied as neuroimaging, transportation networks, and social media use. In these, and many other applications, the relationship between elements of the network (or nodes) can be described by connections (or edges) that capture similarity, coherence, or functionality.² In order to understand these emergent behaviors, we require analytical approaches that respect the relational information between elements of these interacting systems.³

Over the last 6 years, developing novel methods to analyze time-evolving network dynamics of brain activity has been a strong component of the US Army Research Laboratory's (ARL's) ongoing research in translational neuroscience.⁴ This emphasis reflects a theoretical movement from traditional neuroimaging approaches that focused on the computational processing of segregated areas of the brain to a set of innovative network science approaches to investigate the dynamic communication among brain regions.^{5,6} Across the 84 billion neurons in the brain,⁷ networks are dynamically forming and dissolving to connect the localized neural ensembles that perform specialized computational processing as global networks that integrate across regions in support of time-evolving task activity to enable human behavior.^{8,9} Thus, to understand the complex dynamics of neural processing, methods must preserve the spatio-temporal properties that embody what brain regions are communicating and when in intricately timed interaction. The burgeoning field of network neuroscience leverages a graph theoretic approach from network science, where the component parts of a system (nodes) are connected based on their pairwise interactions (edges) in a graph.¹⁰ We will leverage this formalism here since it facilitates the study of brain activity by preserving the underlying geometry of the data. However, since we are interested in time-evolving network dynamics, we cannot rely on traditional approaches that capture scalar signals supported on the nodes of a graph; instead, we consider time-series functions supported on the nodes of a graph.

Graph signal processing has been proposed as a method to analyze functions with an irregular domain that can be described by a weighted graph.^{11,12} These approaches consider scalar functions supported on the vertices of a graph and adapt tools from

classical signal processing such as filtering to account for the graph domain. This work essentially divides into 2 basic approaches: graph Laplacian-based filtering and weighted adjacency matrix-based filtering. In Shuman et al.,¹¹ and elaborated in Bronstein et al.,¹³ filtering operators are polynomials of the graph Laplacian of the graph domain, while in Sandryhaila and Moura,¹² filtering operators are polynomials of the weighted adjacency matrix of the graph domain. At the time of this project, graph Laplacian-based methods have elicited greater use and adoption in the scientific literature and have recently been successfully applied in various deep learning frameworks.¹³

In this report, we assess the possibility of extending the techniques of Shuman et al.¹¹ to the more general problem of time-series functions on the vertices of a fixed weighted undirected graph (see Fig. 1). The rest of the report is outlined as follows. In Section 2, we review the mathematical background necessary for graph signal processing, namely Hilbert spaces, Fourier analysis, and spectral graph theory. In Section 3, we present the graph signal processing approach from Shuman et al.¹¹ In Section 4, we present our original work, extending the approach of Shuman et al.¹¹ to time-series functions on a fixed graph. In Section 5, we discuss the results of this effort. We find that a direct extension of the approach will not generalize to the problem of time-series functions on a graph. Rather, the temporal information that we hope to retain is instead lost because the graph Fourier basis does not form an orthonormal basis for the space of functions in which we are interested. In Section 6, we discuss alternative approaches to address this failure by extending the approach of Sandryhaila and Moura¹² or deliberately constructing an orthonormal basis for the functions.

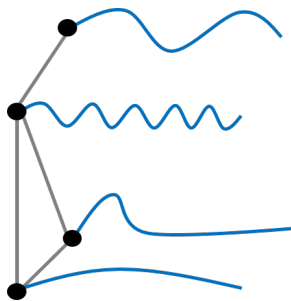


Fig. 1 Time-series function on a fixed graph

2. Mathematical Background

Graph signal processing leverages spectral graph theory to extend classical signal processing operations such as filtering to functions that have irregular domains that can be described by graphs. These methods depend heavily on theory from Hilbert spaces, Fourier analysis, and spectral graph theory. We present here the necessary mathematical background.

2.1 Hilbert Spaces

Hilbert spaces provide the abstract vector space in which functions exist, and it is in this space that the tools of signal processing act on functions. We define some basic definitions relating to Hilbert spaces and provide motivating examples.

Definition 2.1. A *Hilbert space* is a real vector space \mathcal{H} with an *inner product* $\langle f, g \rangle$ such that \mathcal{H} is *complete* in the induced *norm*, $\|f\| = \sqrt{\langle f, f \rangle}$.

Example 2.2. $L^2(\mathbb{R}) = \{f : \mathbb{R} \rightarrow \mathbb{R} \mid \|f\| < \infty\}$, with inner product $\langle f, g \rangle = \int_{-\infty}^{\infty} f(x)g(x)dx$ is an infinite-dimensional Hilbert space.

Definition 2.3. An *orthonormal basis* of a Hilbert space \mathcal{H} is a sequence $\{x_n\}_{n=1}^N$, $N \in \mathbb{N}$, with $\langle x_n, x_m \rangle = \delta_{nm}$ ($\delta_{nm} = 1$ if $n = m$ and 0 otherwise), $\forall n, m \in \mathbb{N}$ such that $x \in \mathcal{H}$ has a unique representation $x = \sum_{n=1}^N \langle x, x_n \rangle x_n$, where x_n are distinct elements.

Example 2.4. The set of functions $\{e^{iwt} : w \in \mathbb{R}\}$ is an orthonormal basis for $L^2(\mathbb{R})$ called the *standard Fourier basis*.

Hilbert spaces make analysis of complicated mathematical objects more intuitive. In a vector space such as \mathbb{R}^n , the canonical basis (i.e., $e_1 = [1, 0, \dots, 0]^T, \dots, e_n = [0, \dots, 0, 1]^T$ where \cdot^T is the usual matrix transpose) forms an orthonormal basis. This construction allows all vectors in the vector space to be represented as linear combinations of a fixed set of canonical vectors. Similarly, the Euclidean distance (i.e., $\|x - y\|^2 = \sum_{i=1}^n x_i y_i$) allows us to measure distance between any 2 vectors in the vector space. Together, these 2 concepts simplify the analysis of vectors. Hilbert spaces generalize these concepts to spaces of functions and other abstract objects. Fourier analysis depends heavily on these concepts to provide an orthonormal basis for arbitrary functions.

2.2 Fourier Analysis

Classical signal processing leverages the results of Fourier analysis to deconstruct functions into simpler trigonometric functions for processing steps such as filtering. We present the definition of the Fourier transform, inverse Fourier transform, and convolution along with the convolution theorem.

A Fourier transform represents a time-series as a linear combination of complex exponential functions in the frequency domain, and the inverse Fourier transform reassembles the frequency components into a time-series. The Fourier transform and inverse Fourier transform provide invertible mappings between the time representation of a signal and the frequency representation of a signal.

Definition 2.5. The *Fourier transform* of a function $f \in L^1(\mathbb{R})$ is defined as

$$\mathcal{F}(f(t)) = \hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t} dt, \quad \text{for } \omega \in \mathbb{R}. \quad (1)$$

Definition 2.6. The *inverse Fourier transform* is defined by

$$\mathcal{F}^{-1}(\hat{f}(\omega)) = f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega)e^{i\omega t} d\omega, \quad \text{for } t \in \mathbb{R}. \quad (2)$$

Implicit in the definition of the Fourier transform is the inner product from $L^2(\mathbb{R})$ and the basis function $e^{i\omega t}$. The Fourier transform is the projection of f onto basis functions indexed by frequency.

The convolution operation provides another basic building block for classical signal processing.

Definition 2.7. A *convolution* operation $* : L^2(\mathbb{R}) \times L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$ is defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} f(y)g(x - y)dy, \quad \text{for } x \in \mathbb{R}. \quad (3)$$

An important property of the convolution is captured in the following, a standard result of Fourier analysis¹⁴ :

Theorem 2.8. (*Convolution Theorem*) *Convolution of two functions in the time do-*

main is equivalent to multiplication in the frequency domain

$$\mathcal{F}[f(t) * g(t)] = \mathcal{F}(f)(w) \cdot \mathcal{F}(g)(w) = \hat{f}(w) \cdot \hat{g}(w). \quad (4)$$

This is a helpful tool in frequency filtering where we choose filter functions (i.e., g in the definition of the convolution) to either amplify or attenuate contributions from the frequency components of a signal (i.e., f in the definition of the convolution). Often, $\hat{g}(\cdot)$ is referred to as the transfer function of the filter, and when combined with the Convolution theorem, filtering can be performed by the following:

$$f_{out}(t) := (f_{in} * g)(t) = \mathcal{F}^{-1}(\hat{f}_{in}(w) \cdot \hat{g}(w)). \quad (5)$$

2.3 Spectral Graph Theory

Graphs provide the topology for arbitrary objects through pair-wise similarity. These relationships build a discrete geometry for data that does not necessarily conform to Euclidean geometry. Spectral graph theory concerns the spectral content (eigenvalues and eigenvectors) of these graphs. Here, we define a graph, review some basic properties, and derive the graph Laplacian and its spectral properties.

Definition 2.9. A *weighted undirected graph* \mathcal{G} is defined as the triple $(\mathcal{V}, \mathcal{E}, \mathcal{W})$, where $\mathcal{V} = \{1, \dots, n\}$ is the set of vertices, $\mathcal{E} = \{\{i, j\} : i, j \in \mathcal{V}\}$ is the set of edges, and \mathcal{W} is the $n \times n$ symmetric adjacency matrix of the edge weights $w_{ij} \geq 0$ for $\{i, j\} \in \mathcal{E}$.

A graph is principally made up of vertices, which represent the objects of interest. We capture relationships between objects by connecting them with edges, where the strength of each edge (the weight) represents the similarity of the connected objects. The pair-wise similarity (or near-ness) of objects induces a unique geometry on the domain. Other common properties of graphs are the degree matrix and neighborhood.

Definition 2.10. The *degree matrix* is defined as $D = \text{diag}(d_1, \dots, d_n)$ where $d_i = \sum_{j: j \neq i} w_{ij}$.

Definition 2.11. The *neighborhood* of a vertex is the set of vertices connected to vertex i by an edge, $\mathcal{N}_i = \{j \in \mathcal{V} | i \neq j, \{i, j\} \in \mathcal{E}\}$.

The neighborhood definition given is general. For our purposes, the neighborhood of a node includes all other nodes in the graph. We can also weight vertices to convey the relative importance of vertices. These weights also become important in developing either the un-normalized or normalized graph Laplacian.

Definition 2.12. The *vertex weight matrix* is defined by $A = \text{diag}(a_1, \dots, a_n)$ where $a_i \geq 0 \in \mathbb{R}$ for all $i \in \mathcal{V}$.

Next, we build spectral graph theory by considering functions defined on a graph. We begin with defining a Hilbert space for these functions.

Definition 2.13. Let $\ell^2(\mathcal{V}) = \{f : \mathcal{V} \rightarrow \mathbb{R} : \|f\|_{\ell^2(\mathcal{V})} < \infty\}$ be the Hilbert space with the following inner product:

$$\langle f, g \rangle_{\ell^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} a_i f_i g_i \quad (6)$$

and induced norm $\|f\|_{\ell^2(\mathcal{V})} = \sqrt{\langle f, f \rangle_{\ell^2(\mathcal{V})}}$.

Definition 2.14. Let $\ell^2(\mathcal{E}) = \{F : \mathcal{E} \rightarrow \mathbb{R} : \|F\|_{\ell^2(\mathcal{E})} < \infty\}$ be the Hilbert space with the following inner product:

$$\langle F, G \rangle_{\ell^2(\mathcal{E})} = \sum_{\{i,j\} \in \mathcal{E}} w_{ij} F_{ij} G_{ij} \quad (7)$$

and induced norm $\|F\|_{\ell^2(\mathcal{E})} = \sqrt{\langle F, F \rangle_{\ell^2(\mathcal{E})}}$.

Then, we use concepts from discrete calculus to define a difference operator that acts on these functions.

Definition 2.15. Let $f \in \ell^2(\mathcal{V})$. The *graph gradient operator* $\nabla : \ell^2(\mathcal{V}) \rightarrow \ell^2(\mathcal{E})$ is defined as

$$(\nabla f)_{ij} = f_j - f_i. \quad (8)$$

Together with the Hilbert space on the edges of the graph, the graph gradient allows us to examine the Dirichlet energy of a function on the graph.

Definition 2.16. The *Dirichlet energy* of $f \in \ell^2(\mathcal{V})$ is defined as

$$S(f) = \frac{1}{2} \|\nabla f\|_{\ell^2(\mathcal{E})}^2. \quad (9)$$

The Dirichlet energy measures the smoothness of functions by summing the gradient (or tendency of the function to change) over the entire domain. This idea is borrowed from statistical physics in which low-energy states are more likely (and more stable) than high-energy states. Importantly, if we define the adjoint of the gradient (∇^*), we can write the Dirichlet energy as a quadratic function of f .

$$\begin{aligned}
S(f) &= \frac{1}{2} \|\nabla f\|_{\ell^2(\mathcal{E})}^2 \\
&= \frac{1}{2} \langle \nabla f, \nabla f \rangle_{\ell^2(\mathcal{E})} \\
&= \frac{1}{2} \langle f, \nabla^* \nabla f \rangle_{\ell^2(\mathcal{E})} \\
&= \frac{1}{2} \langle f, \Delta f \rangle_{\ell^2(\mathcal{E})}
\end{aligned}$$

where $\Delta = D - \mathcal{W}$ is known as the un-normalized graph Laplacian. We note that $S(f) = 0$ if and only if f is constant across all vertices, and $S(f)$ is small when f has similar values at neighboring vertices connected by an edge with a large weight (i.e., when it is smooth).

We may be interested in finding smooth functions $f \in \ell^2(\mathcal{V})$. We know that the subspace of constant functions minimizes the Dirichlet energy, but what about non-trivial functions that minimize the Dirichlet energy? One procedure for finding such functions would be to constrain the subspace of functions to be orthogonal to the subspace of constant functions and minimize the Dirichlet energy within this subspace. We could further ask for another subspace of functions orthogonal to that subspace that minimizes the Dirichlet energy, and repeat this process until we have $|\mathcal{V}|$ orthogonal functions. This procedure can be posed concisely in the following optimization problem:

$$\min_{\Phi \in \mathbb{R}^{n \times n}} \text{tr}(\Phi^T \tilde{\Delta} \Phi) \quad s.t. \quad \Phi^T \Phi = I \quad (10)$$

where $\tilde{\Delta} = A^{-1}(D - \mathcal{W})$ is the un-normalized graph Laplacian if $A = I$ and the normalized graph Laplacian if $A = D$.¹³ This optimization problem is solved by an eigendecomposition of the normalized graph Laplacian, $\tilde{\Delta} = \Phi \Lambda \Phi^T$.

3. Graph Signal Processing

Now that we have established the mathematical tools, we review the approach of Shuman et al.¹¹ to extend classical signal processing tools to functions with a graph domain. We begin with generalizing the Fourier transform and inverse Fourier transform. Then, we use the convolution theorem to define the convolution.

As described in Eq. 1, the Fourier transform is a projection onto an orthonormal basis. This leads us to seek an orthonormal basis for $\ell^2(\mathcal{V})$. We note that the normalized graph Laplacian $\tilde{\Delta}$ is a symmetric matrix, so it has real nonnegative eigenvalues and a complete set of orthonormal eigenvectors that span \mathbb{R}^n . Further, we can associate these eigenvectors with a notion of frequency (or smoothness) because smaller eigenvalues are associated with eigenvectors, or modes, of lower Dirichlet energy. Thus, the eigendecomposition of the graph Laplacian provides us an orthonormal basis for $\ell^2(\mathcal{V})$ that can be partially ordered with respect to frequency (or smoothness). In Shuman et al.,¹¹ associating the Fourier basis with the graph Laplacian eigenbasis provides the means by which we extend signal processing techniques to functions which occur on graphs.

Let $\Phi = [\phi_0, \dots, \phi_{n-1}]$ be the graph Fourier (eigen) basis of the graph Laplacian.

Definition 3.1. The *graph Fourier transform* of a discrete signal $f \in \ell^2(\mathcal{V})$ is defined as

$$\hat{f}_i = \langle f, \phi_i \rangle_{L^2(\mathcal{V})}. \quad (11)$$

Definition 3.2. The *graph inverse Fourier transform* is defined as

$$f = \sum_{i=0}^{n-1} \hat{f}_i \phi_i. \quad (12)$$

Now, we address the convolution. A direct extension is impossible because the definition of the convolution requires a translation operator and such an operation is meaningless on an unordered set of vertices. Therefore, Shuman et al.¹¹ proposes to use the convolution theorem as a definition for the convolution. This bypasses the translation hurdle by using the previously defined Fourier and inverse Fourier transform.

Definition 3.3. The *graph convolution* $*_g : L^2(\mathcal{V}) \times L^2(\mathcal{V}) \rightarrow L^2(\mathcal{V})$ is defined as

$$f *_g g := \sum_{i=0}^{n-1} (\langle f, \phi_i \rangle_{L^2(\mathcal{V})} \langle g, \phi_i \rangle_{L^2(\mathcal{V})}) \phi_i \quad (13)$$

or equivalently,

$$f *_g g = Gf := \Phi \text{diag}(\hat{g}) \Phi^T f, \quad (14)$$

where $\hat{g} = (\hat{g}(\lambda_1), \dots, \hat{g}(\lambda_n))$ is the spectral representation of g .

4. Results

Our problem is such: we want to process signals $\{f_i \in L^2(\mathbb{R})\}_{i \in \mathcal{V}}$ that occur on the vertices of a fixed graph \mathcal{G} . We imagine distinct functions with a fixed spatial topology captured by the graph. Shuman et al.¹¹ considers scalar functions on the vertices of the graph, but here we follow their approach and extend it as necessary to define filtering and convolution operations. We begin with defining the Hilbert space and difference operators for such functions. Then, we compute an orthonormal basis, with which we generalize the Fourier and inverse Fourier transform.

4.1 Hilbert Spaces of Time-Series Signals

Functions on a bounded time domain, $\mathcal{T} = [0, \tau]$, have a natural Hilbert space.

Definition 4.1. Let $L^2(\mathcal{T}) = \{f : \mathcal{T} \rightarrow \mathbb{R} : \|f\| < \infty\}$ be the Hilbert space with the following inner product:

$$\langle f, g \rangle = \int_{\mathcal{T}} f(t)g(t)dt. \quad (15)$$

Here, we consider a set of time-series functions $f = \{f_i \in L^2(\mathcal{T}) : i \in \mathcal{V}\}$. We use the inner product from the Hilbert space for the time domain within the inner product from the graph domain. This provides the following Hilbert spaces:

Definition 4.2. Let $L^2(\mathcal{V} \times \mathcal{T}) = \{f : \mathcal{V} \times \mathcal{T} \rightarrow \mathbb{R} : \|f\| < \infty\}$ be the Hilbert space with the following inner product:

$$\langle f, g \rangle_{L^2(\mathcal{V} \times \mathcal{T})} = \sum_{i \in \mathcal{V}} \left(\frac{a_i}{\tau} \int_{\mathcal{T}} f_i(t)g_i(t)dt \right). \quad (16)$$

Definition 4.3. Let $L^2(\mathcal{E} \times \mathcal{T}) = \{f : \mathcal{E} \times \mathcal{T} \rightarrow \mathbb{R} \mid \|f\| < \infty\}$ be the Hilbert space with the following inner product:

$$\langle F, G \rangle_{L^2(\mathcal{E} \times \mathcal{T})} = \sum_{\{i,j\} \in \mathcal{E}} \left(\frac{w_{ij}}{\tau} \int_{\mathcal{T}} F_{ij}(t) G_{ij}(t) dt \right). \quad (17)$$

4.2 Graph Differential Operators of Time-Series Signals

We follow Bronstein et al.¹³ to define the graph differential operators on the Hilbert spaces $L^2(\mathcal{V} \times \mathcal{T})$ and $L^2(\mathcal{E} \times \mathcal{T})$.

Definition 4.4. The *graph gradient* operator $\nabla_{\mathcal{T}} : L^2(\mathcal{V} \times \mathcal{T}) \rightarrow L^2(\mathcal{E} \times \mathcal{T})$ of a signal $f \in L^2(\mathcal{V} \times \mathcal{T})$ is defined as

$$(\nabla_{\mathcal{T}} f)_{ij}(t) := f_j(t) - f_i(t). \quad (18)$$

Definition 4.5. The *graph divergence* operator $\text{div}_{\mathcal{T}} : L^2(\mathcal{E} \times \mathcal{T}) \rightarrow L^2(\mathcal{V} \times \mathcal{T})$ of a function $F \in L^2(\mathcal{E} \times \mathcal{T})$ is defined as

$$(\text{div}_{\mathcal{T}} F)_i(t) = \frac{1}{a_i} \sum_{j: \{i,j\} \in \mathcal{E}} w_{ij} F_{ij}(t). \quad (19)$$

We verify that the graph gradient is the adjoint of the graph divergence.

Theorem 4.6. *The graph gradient is the adjoint of the graph divergence.*

Proof.

$$\begin{aligned}
\langle F, \nabla_{\mathcal{T}} f \rangle_{L^2(\mathcal{E} \times \mathcal{T})} &= \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau F_{ij}(t) (\nabla f)_{ij}(t) dt \\
&= \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau F_{ij}(t) [f_j(t) - f_i(t)] dt \\
&= \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau F_{ij}(t) f_j(t) dt - \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau F_{ij}(t) f_i(t) dt \\
&= \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ji}}{\tau} \int_0^\tau (-F_{ji}(t)) f_j(t) dt - \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau F_{ij}(t) f_i(t) dt \\
&= \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_0^\tau (-F_{ij}(t)) f_i(t) dt \\
&= \sum_{i \in \mathcal{V}} \frac{1}{\tau} \int_0^\tau \sum_{j: \{i,j\} \in \mathcal{E}} w_{ij} (-F_{ij}(t)) f_i(t) dt \\
&= \sum_{i \in \mathcal{V}} \frac{1}{\tau} \int_0^\tau \frac{1}{a_i} \sum_{j: \{i,j\} \in \mathcal{E}} a_i w_{ij} (-F_{ij}(t)) f_i(t) dt \\
&= \langle -\text{div}_{\mathcal{T}} F, f \rangle_{L^2(\mathcal{V} \times \mathcal{T})}
\end{aligned}$$

We have assumed that F is conservative (i.e., $F_{ij} = -F_{ji}$), as it is in the case of a gradient, and used the symmetry of \mathcal{W} (i.e., $w_{ij} = w_{ji}$).

4.3 Constructing the Graph Fourier Transform

As in spectral graph theory, we can seek the functions that minimize the Dirichlet energy:

$$S_{\mathcal{T}}(f) = \frac{1}{2} \|\nabla f\|_{L^2(\mathcal{E} \times \mathcal{T})}^2 \quad (20)$$

$$= \frac{1}{2} \sum_{\{i,j\} \in \mathcal{E}} \frac{w_{ij}}{\tau} \int_{\mathcal{T}} (\nabla f)_{ij}(t) (\nabla f)_{ij}(t) dt \quad (21)$$

$$= \frac{1}{2\tau} \int_{\mathcal{T}} \sum_{\{i,j\} \in \mathcal{E}} w_{ij} (\nabla f)_{ij}(t) (\nabla f)_{ij}(t) dt \quad (22)$$

$$= \frac{1}{\tau} \int_{\mathcal{T}} \frac{1}{2} \|(\nabla f)(t)\|_{\ell^2(\mathcal{E})}^2 dt \quad (23)$$

$$= \frac{1}{\tau} \int_{\mathcal{T}} S[f(t)] dt \quad (24)$$

The Dirichlet energy for the time-series function is the integral of the instantaneous energy. A similar result is obtained from the orthogonality constraint. Let $\Phi = [\phi_0, \dots, \phi_{n-1}]$ where $\phi_i \in L^2(\mathcal{V} \times \mathcal{T})$ for all $i \in \mathcal{V}$.

$$\langle \phi_i, \phi_j \rangle_{L^2(\mathcal{V} \times \mathcal{T})} = \sum_{k \in \mathcal{V}} \frac{a_k}{\tau} \int_{\mathcal{T}} (\phi_i(t))_k (\phi_j(t))_k dt \quad (25)$$

$$= \frac{1}{\tau} \int_{\mathcal{T}} \sum_{k \in \mathcal{V}} a_k (\phi_i(t))_k (\phi_j(t))_k dt \quad (26)$$

$$= \frac{1}{\tau} \int_{\mathcal{T}} \langle \phi_i(t), \phi_j(t) \rangle_{\ell^2(\mathcal{V})} dt \quad (27)$$

We see that if 2 functions are orthogonal in $\ell^2(\mathcal{V})$ at each time instance, then they are orthogonal in $L^2(\mathcal{V} \times \mathcal{T})$.

In both the objective and constraints of the optimization problem, there is independence over time. The minimum is achieved by instantaneously minimizing the Dirichet energy with respect to the orthogonality constraint. We observe that the graph Fourier basis is obtained by continuously solving an eigenproblem over time.

$$\min_{\Phi(t) \in \mathbb{R}^{n \times n}} \text{tr}(\Phi(t)^T \tilde{\Delta} \Phi(t)) \quad s.t. \quad \Phi(t)^T \Phi(t) = I \quad (28)$$

Furthermore, since \mathcal{G} is not time-varying, $\Phi(t) = \Phi$ is a constant with respect to time.

We can now define our graph Fourier transform:

Definition 4.7. The *graph Fourier transform* of a time-series signal $f \in L^2(\mathcal{V} \times \mathcal{T})$ is defined as

$$\hat{f}_i(t) = \langle f, \phi_i \rangle_{L^2(\mathcal{V} \times \mathcal{T})} \quad (29)$$

$$= \sum_{j \in \mathcal{V}} \frac{a_j}{\tau} \int_{\mathcal{T}} f_j(t) (\phi_i)_j dt \quad (30)$$

$$= \sum_{j \in \mathcal{V}} a_j \left(\frac{1}{\tau} \int_{\mathcal{T}} f_j(t) dt \right) (\phi_i)_j \quad (31)$$

$$= \sum_{j \in \mathcal{V}} a_j \bar{f}_j (\phi_i)_j \quad (32)$$

$$= \langle \bar{f}, \phi_i \rangle_{\ell^2(\mathcal{V})} \quad (33)$$

where we use $\phi_i(t) = \phi_i$ for all $i \in \mathcal{V}$ and $t \in \mathcal{T}$ and \bar{f} is the average of f over \mathcal{T} .

Definition 4.8. The *graph inverse Fourier transform* of a time-series signal \hat{f} is defined as

$$f(t) = \sum_{i=0}^{n-1} \frac{1}{\tau} \int_{t \in \mathcal{T}} \hat{f}_i(t) \phi_i dt. \quad (34)$$

4.4 Graph Convolution for Time-Series Signals

Finally, we can construct the convolution as done in Shuman et al.¹¹

Definition 4.9. The *graph convolution* $*_{\mathcal{T}} : L^2(\mathcal{V} \times \mathcal{T}) \times L^2(\mathcal{V} \times \mathcal{T}) \rightarrow L^2(\mathcal{V} \times \mathcal{T})$ is defined as:

$$f *_{\mathcal{T}} g := \sum_{i=0}^{n-1} (\langle f, \phi_i \rangle_{L^2(\mathcal{V} \times \mathcal{T})} \odot \langle g, \phi_i \rangle_{L^2(\mathcal{V} \times \mathcal{T})}) \phi_i. \quad (35)$$

5. Discussion

There is a fundamental problem in this construction of the convolution. The convolution theorem depends on the invertibility of the Fourier transform by the inverse Fourier transform. However, we observe a loss of information through the proposed graph Fourier transform. Let us consider a function $f \in L^2(\mathcal{V} \times \mathcal{T})$. Given its spectral representation \hat{f} , we should be able to recover f exactly by the inverse graph Fourier transform.

$$f(t) \stackrel{?}{=} \sum_{i=0}^{n-1} \frac{1}{\tau} \int_{t \in \mathcal{T}} \hat{f}_i(t) \phi_i dt \quad (36)$$

$$\stackrel{?}{=} \sum_{i=0}^{n-1} \frac{1}{\tau} \int_{t \in \mathcal{T}} (\langle f, \phi_i \rangle_{L^2(\mathcal{V} \times \mathcal{T})}) \phi_i dt \quad (37)$$

$$\stackrel{?}{=} \sum_{i=0}^{n-1} \frac{1}{\tau} \int_{t \in \mathcal{T}} (\langle \bar{f}, \phi_i \rangle_{\ell^2(\mathcal{V})}) \phi_i dt \quad (38)$$

$$\stackrel{?}{=} \sum_{i=0}^{n-1} \langle \bar{f}, \phi_i \rangle_{\ell^2(\mathcal{V})} \phi_i \quad (39)$$

$$\neq \bar{f} \quad (40)$$

Instead, we simply recover the average of f over time.

This result is not only unsatisfying but also wholly insufficient. We set out to treat the time domain simultaneously with the irregular spatial domain, but in doing so, we ultimately still lost all but first-order information in the time domain. We can now recognize that this straight-forward extension of the approach in Shuman et al.¹¹ did not result in the construction of an orthonormal basis as in the case of scalar functions on a fixed graph. $\{\phi_i\}_{i \in \mathcal{V}}$ does not span $L^2(\mathcal{V} \times \mathcal{T})$, a necessary condition for the Fourier transform to be invertible.

6. Conclusion

We have evaluated the possibility of extending the approach proposed in Shuman et al.¹¹ for signal processing of scalar functions supported on a fixed graph domain to the case of time-series functions supported on a fixed graph domain. Following a similar construction of the Fourier and inverse Fourier transform and convolution operations, the result is insufficient. All but first-order information from the temporal domain is lost within the convolution. A straight-forward extension of the approach failed to yield an orthonormal basis, but this points to a path forward.

Our future work will investigate 2 alternative approaches. In the first, we will investigate extending the approach proposed in Sandryhaila and Moura¹² where time-series signals (discretely sampled functions) can be considered directed graphs in which time samples can be represented by nodes that are connected only to adjacent time samples in a directed (causal) manner. In the second, we will consider methods that yield an orthonormal basis by design. We recognize that these time-series functions exist in a Hilbert space that is itself the composition of Hilbert spaces with known orthonormal bases. We want to use Fourier basis functions to represent the temporal information in our functions while retaining the spatial basis functions that capture the geometry of our domain. Thus, we could use constructive techniques to deliberately assemble an orthonormal basis for this Hilbert space of time-series functions on graphs by considering functions from either a direct sum (i.e., $L^2(\mathcal{V} \times \mathcal{T}) = L^2(\mathcal{T}) \oplus \dots \oplus L^2(\mathcal{T})$) or tensor product (i.e., $L^2(\mathcal{V} \times \mathcal{T}) = \ell^2(\mathcal{V}) \otimes L^2(\mathcal{T})$) of Hilbert spaces.

Immediate future applications will focus on the analysis of neuroimaging data using these graph signal processing approaches. This approach provides an opportunity to identify novel spatio-temporal features of the data that provide insight about the underlying brain network dynamics. While these features in and of themselves may

have interesting interpretation within the field of network neuroscience, they can also be used in conjunction with machine learning approaches to identify brain dynamics that can predict fluctuations in performance, providing an opportunity to advance the state-of-the-art from previous ARL research.¹⁵⁻¹⁸ More generally, this approach is not limited to applications on neuroimaging data, and it can also provide important contributions to understanding time-evolving network across a host of additional Army-relevant domains, including diverse domains such as communication networks, sensor networks, and social networks.

7. References

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